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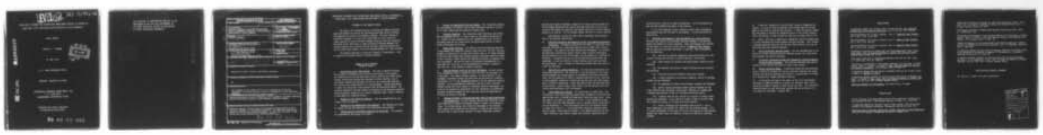

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SEMIDIRECT METHODS FOR DISCRETIZED NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS, WITH PARTICULAR APPLICATIONS TO FLUID DYNAMICS

FINAL REPORT

PATRICK J. ROACHE

15 MAY 1979

U. S. ARMY RESEARCH OFFICE

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ECODYNAMICS RESEARCH ASSOCIATES, INC.
P. O. BOX 8172
ALBUQUERQUE, NEW MEXICO 87198

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Semidirect methods utilize direct (non-iterative) linear solvers to solve nonlinear problems in a non-time-like iteration. The semidirect methods are applied to various fluid dynamics problems. In each case, the direct linear solver used is some variation of a marching method.

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SEMIDIRECT METHODS FOR DISCRETIZED NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS, WITH PARTICULAR APPLICATIONS TO FLUID DYNAMICS

STATEMENT OF THE PROBLEM STUDIED

The scope of the contract work was to develop and improve efficient semidirect methods for solving the discretized nonlinear partial differential equations of various fluid dynamics problems. The basic concept of "semidirect" methods is to use direct (non-iterative) fast solvers for linear equations to solve nonlinear problems using non-time-like iterations. The direct solver used herein is some variation of marching methods; the research progress thus involved both the nonlinear semidirect methods and the tool which these require, the direct marching methods for linear problems.

The proposal described 12 particular avenues of investigation. Each of these will be covered briefly in the next section.

SUMMARY OF MOST IMPORTANT TECHNICAL RESULTS

1. <u>Fourth-Order Driver (FOD) Methods</u>. This type of semidirect method was successfully developed, but not quite as envisioned in the proposal. The intention was to use the Bauer-Reiss block-5 code for the linear solver. Instead, the marching methods were extended to block-5 matrices, and an even better approach was developed solving the two second-order equations for vorticity and stream function in a coupled manner. The marching method is faster and allows much larger problems than the Bauer-Reiss method. The resulting semidirect nonlinear method is preferable to the previous sequential-equation approach, especially for strongly separated flows, since it requires no semi-empirical relaxation factors.

2. <u>Methods for the Primitive Equations</u>. This was accomplished as anticipated, with no surprises.

3. <u>Methods for the Compressible Flow Equations</u>. This approach was proven in concept, but was not exercised in any interesting flow problems.

4. <u>Methods Based on Third-Order Equations for Velocities</u>. This approach was superceded by the success of #1 above.

5. Viscous 1-D Compressible Flow with Shocks. This interesting problem was unfortunately not studied, due to time limitations and due to a priority of other interesting and successful problem areas.

6. Transonic Equations. This problem has been formulated, and we have made arrangements with Dr. M. Hafez to work on the physical problem with us. However, we have postponed the final implementation until we have a structured code for the linear solver including stabilization, so that a highly refined mesh can be used.

7. Higher Order Solutions. The deferred correction approach described in the proposal was tested and proven to work quite well for $O(\Delta^4)$ accuracy. Attempts to achieve $O(\Delta^6)$ accuracy have failed, even in 1-D linear problems. It has also been learned that gradient boundary conditions should be solved to $O(\Delta^4)$ directly, rather than by the deferred correction, to enhance iterative convergence. We have not found a satisfactory implementation of a high-order wall vorticity in the coupled-equation approach, although it does work well in the sequential-equation approach.

8. Improved Boundary Vorticity for Split NOS Method. We have successfully implemented Israeli's method for wall vorticity, and extended it to a high order. This method improves accuracy, is easily applied in non-orthogonal coordinate systems, and simplifies the evaluation of iterative convergence, so it is now recommended generally for the sequential-equation approach. We also experimented extensively with multi-level iteration methods and met with minor success in improving iterative convergence, but primarily we developed an appreciation for the limitations of conventional one-point iteration schemes for wall vorticity, which are superceded by #1 above for difficult problems.

9. Improved Estimates of Advanced Nonlinear Terms by Quasilinearization and Extrapolation. We just recently realized the limitation on any quasilinearization (generalized Newton) method in regard to the operation count. For an MxM problem, even iterative improvement of the Jacobian would require $O(M^3)$ operations per iteration, so that we have settled on the Split NOS or quasi-Picard iteration for multi-dimensional problems.

Gartling has recently performed a comparison of these iteration schemes for finite element methods and has come to the same conclusion; he also finds the Split NOS method less sensitive than Newton iteration to initial guesses, especially at high Re. For 1D problems, Newton iteration is clearly superior.

Unfortunately, we have not found time to experiment with extrapolation of the nonlinear coefficients.

10. Turbulence Equations, Non-Newtonian Fluids, and Temperature-Dependent Viscosities. The generic equation for all these is a nonlinear diffusion term, typified by a turbulence equation using a simple eddy viscosity formulation. This equation has been successfully implemented. As expected, the additional nonlinearity caused slightly slower iterative convergence and more sensitivity to the initial guess, but the method still performs excellently. A pleasant surprise, easily analyzed and predicted after the experiment, is that the addition of eddy viscosity stabilizes the linear marching method. Also, a method for predicting optimum under-relaxation at a wall was developed.

11. Application to Complex Geometries. This has been accomplished with considerable generality. The inclusion of cross-derivatives in the linear marching methods has allowed general non-orthogonal coordinate transformations, and the extension of Israeli's boundary condition for wall vorticity to non-orthogonal systems has allowed high accuracy with even some improvement in iterative convergence. Codes have been written and exercised which allow arbitrary tabular input of wall shape, with the necessary wall derivatives being obtained by $O(\Delta^6)$ differences.

12. Three-Dimensional Problems. The success here has been mixed. The limitations of the direct marching method simply extended to 3D (3D EVP) has been defined, with a 15x15x30 grid emerging as about the upper limit. Also, the speed is not nearly as favorable as in 2D. A very successful 3D EVP/FFT linear solver has been developed, using a Discrete Fourier Transform in the 3rd coordinate, z. This unfortunately restricts the equation solved to terms like $\partial^2/\partial z^2$ in z. In the semidirect iteration, advection terms must be lagged. Under separate funding, it was demonstrated that the nonlinear iterations using several schemes were unstable, apparently due to

the sensitivity of the FFT to small perturbations. The 3D performance has been the most disappointing aspect of the research.

As is to be expected in basic research, several other developments occurred which were not outlined in the proposal. A brief description of these follow.

13. Additional Developments in Marching Methods for Linear Equations. The basic tool used for the nonlinear semidirect methods is the marching method (EVP method) for linear equations. Major developments were achieved and described in a three-part review article in Numerical Heat Transfer. Some of these have been described above; in addition, other developments are indicated here.

13A. Accurate and complete operations counts were derived and a 30% (typical) savings was realized by avoiding some null calculations.

13B. Stable methods for gradient and mixed boundary conditions were developed.

13C. The destabilizing effect of upwind differencing was discovered and explained.

13D. Cross-derivatives and Helmholtz terms were included.

13E. A simple expression of previously graphical results for maximum problem size was developed.

13F. An expanding grid based on the Fibonacci sequence was developed.

13G. Several rapidly converging global-iterative methods for the linear equations were developed, using direct solutions on a submesh and/or banded approximations to the full influence coefficient matrix.

13H. A general code for the solution of a 9-point or 5-point linear operator was developed. It was used by M. Luther of UNC on the CRAY computer at NCAR this spring, on an ocean circulation problem.

13I. Several techniques were developed (both by the P.I. and by other researchers) and compared for stabilizing the marching methods. This is a major development in the state of the art, and promises to make marching methods into robust tools for numerical solutions of physically important problems.

14. A peculiar instability in the Split NOS iteration scheme was discovered. It arose for high Re separated flow problems when the initial guess on the velocity field was too accurate. A stability analysis showed that the method is unstable at stagnation points in the initial velocity field; the problem is simply avoided by requiring a minimum value of $|V^0|$.

15. With D. Gartling, a comparison of semidirect iteration schemes used in finite difference and finite element solutions was made. This included a thorough operation count not only for the linear solution, but also for the entire nonlinear solution procedure.

16. Vorticity-Velocity Equation System. Like the implementation of the primitive variable (pressure-velocity) equation system, this application was successful and held no surprises.

17. Cylindrical Coordinate Problem with Exponential Coordinate Mapping and Rezone Mesh Refinement. This code was developed under partial funding of this contract and partially under a BRL contract.

18. Natural Convection Method. A semidirect method has been developed which is especially suitable for natural convection problems; the stream function and vorticity equations are solved in a coupled manner, followed by a (sequentially) lagged temperature equation.

19. An evaluation was made of the papers at the First International Conference on Numerical Methods in Laminar and Turbulent Flows, held at University College of Swansea in Wales during July 1978. This evaluation focused primarily on work being done overseas, and was written up in a trip report for ARO dated 15 January 1979.

PUBLICATIONS

"A Semidirect Method for Internal Flows in Flush Inlets", Proc. AIAA 3rd Computational Fluid Dynamics Conference, June 27-28, 1977, pp. 149-155.

"Marching Methods for Elliptic Problems: Part 1", Numerical Heat Transfer, Vol. 1, No. 1, pp. 1-15, 1978.

"Marching Methods for Elliptic Problems, Part 2", Numerical Heat Transfer, Vol. 1, No. 2, pp. 163-181.

"Marching Methods for Elliptic Problems, Part 3", Numerical Heat Transfer, Vol. 1, No. 2, pp. 183-201.

"Semidirect Calculation of Steady Two- and Three-Dimensional Flows", Proc. First Inter. Conf. on Numerical Methods in Laminar and Turbulent Flows, Pentech Press, London, pp. 17-28.

"Efficiency Trade-offs of Steady-State Methods Using FEM and FDM", (with D. K. Gartling), ibid, pp. 103-112.

"Preliminary Investigation of the Singular Behavior of Fluids Near a Sliding Corner", (with C. Zoltani), to appear in Proc. 1979 Army Numerical Analysis and Computers Conference, 14-16 February 1979, El Paso, TX.

"A Semidirect Method with Non-Iterative Boundary Coupling for Viscous Flows", to appear in Computers & Fluids.

"A Semidirect Method Suitable for Recirculating Flows Driven by Bouyancy and Shear", to appear in Proc. Inter. Conf. on Numerical Methods in Thermal Problems, 2-6 July 1979, Univ. College, Swansea, Wales.

Semidirect Methods in Fluid Dynamics, Springer-Verlag, to appear.

PRESENTATIONS

"Direct Solution of Variable Coefficient Elliptic Equations Including First and Cross-Derivatives", SIAM National Meeting, Chicago, Ill., June 1976.

"A Semidirect Method for Internal Flows in Flush Inlets", AIAA Third Computational Fluid Dynamics Conference, Albuquerque, New Mexico, June 1977.

Direct Solution of Variable Coefficient Elliptic Equations in Three Dimensions, SIAM 1977 Fall Meeting, Albuquerque, New Mexico, October 1977.

"Semidirect Calculation of Steady Two- and Three-Dimensional Flows", First Inter. Conf. on Numerical Methods in Laminar and Turbulent Flows, Univ. College, Swansea, Wales, July 1978.

"Efficiency Trade-offs of Steady-State Methods Using FEM and FDM", (with D. K. Gartling), ibid.

"Preliminary Investigation of the Singular Behavior of Fluids Near a Sliding Corner", (with C. Zoltani), 1979 Army Numerical Analysis and Computers Conference, 14-16 February 1979, El Paso, TX.

"Semidirect Methods for the Steady-State Navier-Stokes Equations", Seminar at Dept. of Engineering Science and Mechanics, Univ. of Tennessee, Knoxville, Tenn., 7 May 1979.

"A Semidirect Method with Non-Iterative Boundary-Coupling for Viscous Flows", to be presented at Conference on Computers in Aerodynamics, Polytechnic Institute of New York, 4-5 June 1979.

"A Semidirect Method Suitable for Recirculating Flows Driven by Bouyancy and Shear", to be presented at Inter. Conf. on Numerical Methods in Thermal Problems, 2-6 July 1979, Univ. College, Swansea, Wales.

PARTICIPATING TECHNICAL PERSONNEL

Dr. Patrick J. Roache, Principal Investigator.